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A non-statistical atomic model for beam emission and motional Stark effect diagnostics in fusion plasmas[a)]

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In this work we analyze magnetic sublevel populations in a neutral beam penetrating a fusion plasma. The collisional-radiative model NOMAD was extended to include magnetic parabolic sublevels with principal quantum numbers $n \leq 10$. The collisional parameters were calculated with the advanced atomic-orbital close coupling method and the Glauber approximation. The ionization by the induced electric field was also included in the model. The results of our calculations show significant deviations of the sublevel populations and, accordingly, line intensities of the σ and π components, from the statistical approximation. It is shown, for instance, that for a number of experimental conditions the total intensity of σ components is not equal to the total intensity of π components, which has a strong effect on determination of magnetic field and pitch angle in fusion devices. The results are presented for a wide range of plasma and beam parameters. The most significant deviations are observed for strong magnetic fields and high beam energies typical for the ITER plasma, where component intensity ratios may deviate by more than 20% from the statistical values. © *2012 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4728093]

I. INTRODUCTION

The highly energetic beams of neutral particles (primarily hydrogen and deuterium) are extensively used for heating and diagnosis of fusion plasmas. The tokamak ITER, which is currently under construction in Cadarache, France will utilize two powerful (500 keV/u) neutral beam injectors for plasma heating, and another beam with the energy of 100 keV/u will be used for diagnostic purposes. Neutral beams are also implemented on various existing fusion devices, for instance, JET, TEXTOR, and Alcator C-Mod. It is therefore important to provide a reliable theoretical support to the beam-related experimental techniques including such well-known methods as charge-exchange recombination spectroscopy and motional Stark effect (MSE).[1,2]

One of the key issues in beam emission studies and MSE diagnostics is the adequate description of the beam excited state populations. The structure of a neutral atom under the influence of the strong induced electric field $F = v \times B$ (v is the beam velocity and B is the magnetic field in a fusion device) is different from the field-free case: the eigenstates of hydrogen atom are the parabolic states (nkm) rather than the spherical states (nlm), where n is the principal quantum number, k is the electric quantum number,[3] l is the angular momentum, and m is its projection onto z axis (magnetic number). This feature greatly complicates development of collisional-radiative (CR) models for determination of (sub-)level populations since all calculations of collisional parameters (such as cross sections and rate coefficients) are performed for isolated, field-free atoms. It is due to this complication that most of the existing CR models assume the statistical (Boltzmann) distribution for sublevels with the same n:

$$\frac{N_a}{N_b} = \frac{g_a}{g_b}, \tag{1}$$

where N_a is the population of the sublevel a and g_a is its statistical weight. However, numerous experimental data on MSE spectra from JET and other devices clearly point out to a strong deviation from the statistical approximation. This problem calls for a detailed analysis of validity of the statistical method in neutral beam diagnostics.

II. COLLISIONAL-RADIATIVE MODEL FOR PARABOLIC STATES

To analyze the population distributions among the excited states of the neutral beam particles, we use the CR model NOMAD.[4] This model was extended, as compared to our previous simulations,[5] to include 210 parabolic (nkm) states in neutral hydrogen with $n \leq 10$. The energies and radiative rates were determined using perturbation theory[3] while the exact quantummechanical results[6] were used for the field-induced ionization rates.

Since the collisional energies are on the order of tens and hundreds of keV/u, the most important collisional processes for the present modeling are the proton-impact transitions (mainly excitations) between the hydrogen states. We recently developed a new approach[5] to calculation of collisional cross

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sections between magnetic sublevels and the reader is referred to the original publication for the details. In this method, the cross sections between magnetic *parabolic* states are represented as the linear combinations of the diagonal (i.e., cross sections) and off-diagonal elements of the density matrix for transitions between magnetic *spherical* states. This allows one to implement the well-developed standard collisional methods for calculation of scattering amplitudes. For the present work, we performed calculations of proton-impact excitations using the atomic-orbital close coupling method[7] and the Glauber approximation.[8] The calculated collisional parameters were compared with other available results[9,10] and generally a good agreement was found, especially for high beam energies above 100 keV/u.

The parabolic state populations were calculated using the time-dependent system of rate equations

$$\frac{d\hat{N}(t)}{dt} = \hat{A} \cdot \hat{N}(t), \tag{2}$$

where $\hat{N}(t)$ and $\hat{A}$ are the state population vector and the rate matrix, respectively. At $t = 0$ all population was in the ground state, and integration of system (2) continued until about 100 ns when excited states reach quasi-steady-state equilibrium. The simulations were performed in a wide range of plasma densities, from 10^{10} cm^{-3} to 10^{16} cm^{-3}, and for beam energies between 50 keV/u and 500 keV/u with the magnetic field of 3 T to 5 T.

An example of the calculated results for relative populations $n_i \equiv N_i/g_i$ is presented in Fig. 1. The top panel shows n_i for $2 \le n \le 9$ calculated without field-induced ionization (FII) at the particle density of 3×10^{13} cm^{-3}, the beam energy of 50 keV/u, and the magnetic field of 3 T, while the bottom panel results do include FII for the same plasma conditions. Even without the FII, the populations of the $n = 3$ levels are seen to deviate from the statistical distribution, which corresponds to a horizontal line. This is due to the relatively strong radiative processes as compared to the collisional ones. Only for high principal quantum numbers, $n \ge 8$, the populations become practically statistical. For the FII simulations shown in Fig. 1(b), the high-n populations are very different from the statistical limit since the ionization due to the induced electric field efficiently destroys the Boltzmann distribution of populations. It is also clear that the deviation from the statistical distribution increases for mid-n states with $n \approx 5$ due to collisional coupling with the high-n states.

It would be rather difficult to introduce a simple and straightforward parameter to provide an unambiguous criterion for the statistical distribution for (nkm) states. The energies of these states are different for different combinations of beam velocity and magnetic field strength, and the collisions between slow plasma particles and fast neutrals are not Maxwellian. Even more important is the field-induced ionization, which becomes a strong and uncompensated depopulation channel, especially for high-n states. It is possible, of course, to introduce a quantity that can "measure" deviations from the Boltzmann distribution. For instance, one can use the standard deviation of reduced populations from the statistical limit defined as

$$\zeta_n = \sqrt{\frac{1}{M} \cdot \sum_{i=1}^{M} \left(\frac{n_i}{\overline{n}} - 1\right)^2}, \tag{3}$$

$$\overline{n} = \frac{\sum_j N_j}{\sum_j g_j}, \tag{4}$$

where summations in both equations go over magnetic parabolic states within a specific n, $M = n(n + 1)/2$ is the number of parabolic levels within the n state and $\overline{n}$ is the averaged (non-reduced) population for the states with a principal quantum number n. Obviously, the parameter ζ_n becomes zero for the statistical distribution. In Fig. 2 the calculated values of ζ_n with (solid lines) and without (dashed lines) collisional and field ionization for $n = 2-4$ are

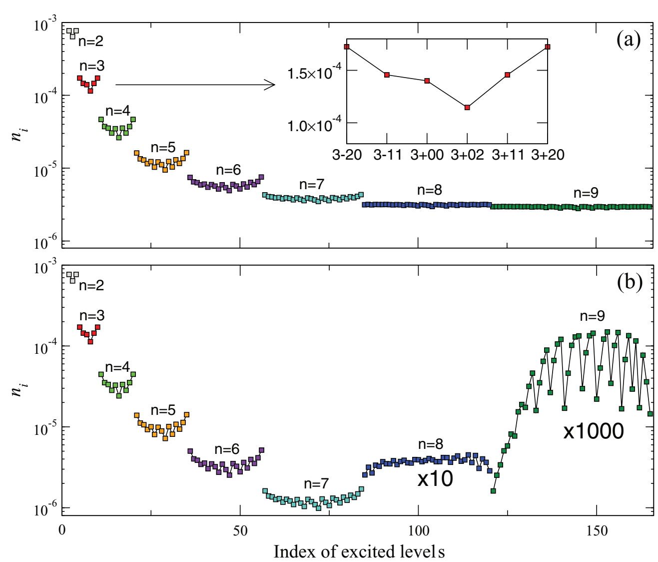

FIG. 1. Reduced populations for the hydrogen parabolic states (nkm) arranged according to the energy within the same n. The beam energy is 50 keV/u, the plasma temperature and density are 3 keV and 3×10^{13} cm^{-3}, and the magnetic field is 3 T. The inset presents the $n = 3$ parabolic state populations on a linear scale.

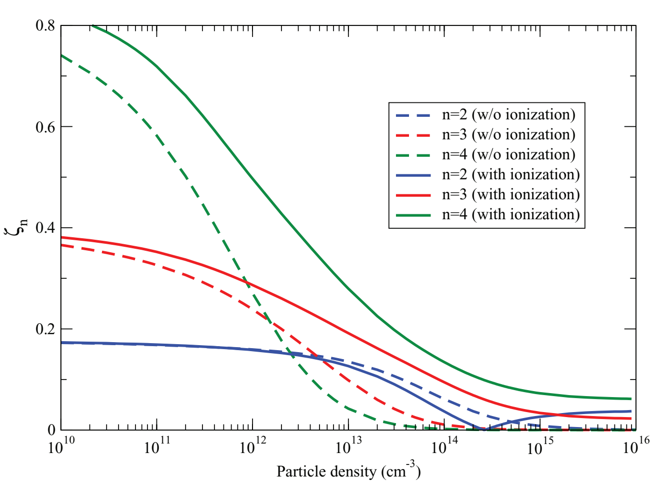

FIG. 2. Parameter ζ_n calculated for the beam energy of 50 keV/u, the plasma temperature of 3 keV, and the magnetic field of 3 T. The calculations without collisional and field ionization are shown by dashed lines, and calculations with ionization are shown by solid lines.

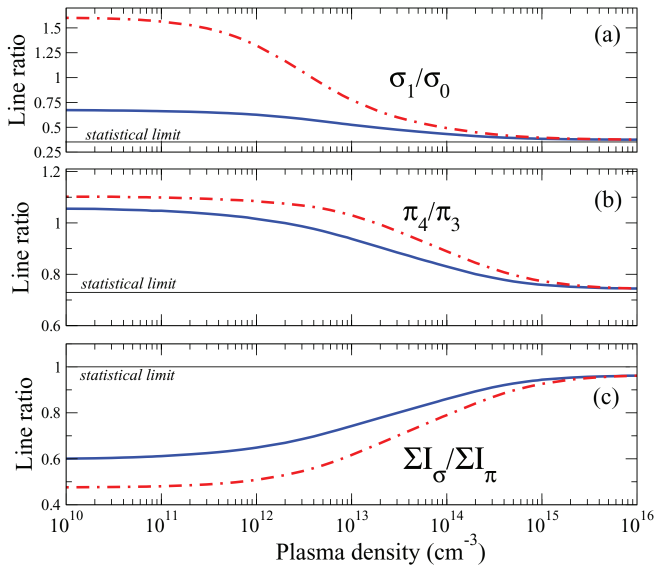

FIG. 3. Ratios of H_α components and total σ and π emissions as functions of particle density at magnetic field of 5 T. The beam energies are 100 keV/u (solid lines) and 500 keV/u (dotted-dashed lines). The statistical limits are shown by thin horizontal lines.

presented as a function of particle density for a 50 keV/u beam in a 3 keV plasma with the magnetic field of 3 T. Without ionization, the populations approach the statistical results in the high-density limit. For a complete calculation including collisional and field ionization, the density dependence of ζ_n changes drastically, and the statistical limit is not achieved at high densities for any n with $\zeta_n \approx 5\%–10\%$. At the typical fusion plasma density of 5×10^{13} cm^{-3}, ζ_n is on the order of 15% for $n = 3$ and larger for $n = 4$. Since this parameter is an averaged quantity, the actual deviations between different sublevels and, consequently, different components of a spectral multiplet, may be much larger. Note also that the vanishing ζ_2 at approximately 2×10^{14} cm^{-3} is the result of coincidence of populations for (2, ±1, 0) and (2, 0, 1) substates.

Finally, in Fig. 3 we present the particle density dependence of the calculated ratios for the strongest components of H_α Stark multiplet, σ_1/σ_0 and π_4/π_3, as well as the ratio of the total σ and π intensities. The magnetic field in this calculation was taken to be 5 T and the beam energies were 100 keV/u and 500 keV/u. The deviation from the statistical limits, shown by horizontal lines, strongly increases for low densities so that for instance, unlike the statistical limit, the σ_1 component becomes stronger than σ_0. Also, at typical fusion plasma densities the total σ component intensity is about 20% weaker than the total π intensity while the statistical limit is 1.

III. CONCLUSIONS

Since a number of important parameters related to neutral beam diagnostics in fusion plasmas crucially depend on populations of excited states, development of reliable atomic models becomes an important topic in fusion research. Unlike isolated atoms, the structure of the neutral beam particles in a magnetically confined plasma is strongly affected by the induced electric field so that their eigenstates are parabolic rather than spherical states. Although this feature brings about extra complications for calculation of the relevant collisional parameters, the recently developed methods allow one to generate all required data sets for collisional-radiative modeling of neutral beam emission including motional Stark effect.

In this paper we implemented an extensive CR model for analysis of non-statistical effects in sublevel populations. Our calculations in a wide range of plasma and beam parameters show that the parabolic states of a hydrogen beam cannot be described in the statistical approximation due to the strong radiative decays and the field-induced ionization. We introduced a new parameter to describe deviations from the Boltzmann distribution. Also we presented the calculated ratios of σ and π components of H_α Stark multiplet. These results can be used for plasma diagnostics in existing and future fusion devices including ITER.

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